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THE FAST INVARIANT IMBEDDING METHOD FOR POLARIZED LIGHT: COMPUTATIONAL ASPECTS AND NUMERICAL RESULTS FOR RAYLEIGH SCATTERING

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Abstract—Computation of the reflection matrix for a finite, plane-parallel, vertically-inhomogeneous, isotropic atmosphere is considered. The fast invariant imbedding method of Sato, Kawabata, and Hansen is extended to include polarization. Computational aspects of this extension are discussed in detail, and numerical results are presented for the angular distribution of polarized radiation reflected by an atmosphere with Rayleigh scattering and an exponentially-varying albedo for single scattering.

1. INTRODUCTION

Sato et al[1] have proposed an efficient method (hereafter referred to as the fast invariant imbedding method) to calculate the intensity of light reflected by a plane-parallel slab of finite optical thickness. The method is based on a special predictor–corrector scheme for solving the invariant imbedding equation for a Fourier-decomposed reflection function. They showed that for atmospheres with continuously-varying optical properties, the fast invariant imbedding method becomes substantially more efficient than the commonly used adding/doubling method.

The main purpose of the present paper is to extend the fast invariant imbedding method to include polarization, i.e., to treat the albedo problem using the full (4×4) reflection matrix instead of the reflection function. As was noted by De Haan et al,[2] this extension is in principle straightforward, but should not be restricted only to replacing scalar quantities by the corresponding matrices if a concise and efficient computer code is desired. We present some illustrative numerical results for the classical problem of Rayleigh scattering. Finite slabs will be considered with an exponentially-varying albedo for single scattering.

2. BASIC FORMULAE AND EQUATIONS

To describe the state of polarization of light, we use the intensity vector $\mathbf{I}$, which has four Stokes parameters as its components as follows:

$$\mathbf{I} = \begin{bmatrix} I \\ Q \\ U \\ V \end{bmatrix}. \tag{1}$$

For a plane-parallel, isotropic, vertically-inhomogeneous atmosphere of optical thickness t, the direction of light incident on or reflected by the atmosphere will be specified by the cosine of the angle between the direction of light propagation and the normal to the boundaries of the atmosphere $\mu (0 \leqslant \mu \leqslant 1)$ and by the azimuth angle φ. The upper boundary of the atmosphere is illuminated by a parallel beam of light, which is specified by the intensity vector $\pi \mathbf{F} \delta(\mu - \mu_0) \times \delta(\varphi - \varphi_0)$ where δ is the Dirac delta function; also $\mathbf{I}(t; \mu, \mu_0, \varphi - \varphi_0)$ is the intensity vector of light reflected by the atmosphere. Expanding $\mathbf{I}(t; \mu, \mu_0, \varphi - \varphi_0)$ in a Fourier series, we have

$$\mathbf{I}(t; \mu, \mu_0, \varphi - \varphi_0) = \sum_{m=0}^{\infty} (2 - \delta_{m0})[\mathbf{I}_c^m(t; \mu, \mu_0)\cos m(\varphi - \varphi_0) + \mathbf{I}_s^m(t; \mu, \mu_0)\sin m(\varphi - \varphi_0)], \tag{2}$$

where δ_{ij} is the Kronecker delta.

Following Refs. 3–5, we write

$$\mathbf{I}_c^m(t;\mu,\mu_0)=\tfrac{1}{2}(\mathbf{E}+\mathbf{D})\mathbf{I}_m^+(t;\mu,\mu_0)+\tfrac{1}{2}(\mathbf{E}-\mathbf{D})\mathbf{I}_m^-(t;\mu,\mu_0), \tag{3}$$

$$\mathbf{I}_s^m(t;\mu,\mu_0)=\tfrac{1}{2}(\mathbf{E}-\mathbf{D})\mathbf{I}_m^+(t;\mu,\mu_0)-\tfrac{1}{2}(\mathbf{E}+\mathbf{D})\mathbf{I}_m^-(t;\mu,\mu_0), \tag{4}$$

$$\mathbf{I}_m^\pm(t;\mu,\mu_0)=\mu_0\mathbf{R}^m(t;\mu,\mu_0)\mathbf{F}^\pm, \tag{5}$$

where $\mathbf{E}$ is the (4×4) unit matrix,

$$\mathbf{D}=\mathrm{diag}(1,1,-1,-1), \tag{6}$$

$$\mathbf{F}^\pm=\tfrac{1}{2}(\mathbf{E}\pm\mathbf{D})\mathbf{F}. \tag{7}$$

The (4×4) matrices $\mathbf{R}^m(t;\mu,\mu_0)$ are solutions of the invariant imbedding equation

$$\begin{aligned}\frac{\mathrm{d}\mathbf{R}^m(t;\mu,\mu_0)}{\mathrm{d}t}=&-\left(\frac{1}{\mu}+\frac{1}{\mu_0}\right)\mathbf{R}^m(t;\mu,\mu_0)+\frac{w}{4\mu\mu_0}\mathbf{Z}^m(-\mu,\mu_0)\\&+\frac{w}{2\mu_0}\int_0^1\mathrm{d}\mu'\mathbf{R}^m(t;\mu,\mu')\mathbf{Z}^m(\mu',\mu_0)\\&+\frac{w}{2\mu}\int_0^1\mathrm{d}\mu'\mathbf{Z}^m(-\mu,-\mu')\mathbf{R}^m(t;\mu',\mu_0)\\&+w\int_0^1\int_0^1\mathrm{d}\mu'\,\mathrm{d}\mu''\mathbf{R}^m(t;\mu,\mu')\mathbf{Z}^m(\mu',-\mu'')\mathbf{R}^m(t;\mu'',\mu_0),\end{aligned} \tag{8}$$

which describes how the reflection matrix is changed when a new, optically-thin layer, which is specified by the single scattering albedo w and by the matrices $\mathbf{Z}^m$ is added to the top of the atmosphere. Equation (8) is supplemented by the initial condition

$$\mathbf{R}^m(0;\mu,\mu_0)=\mathbf{R}^m(\mu,\mu_0). \tag{9}$$

The (4×4) matrices $\mathbf{Z}^m$ are defined by[3–5]

$$\mathbf{Z}^m(u,u')=(-1)^m\sum_{s=m}^{\infty}\mathbf{P}_m^s(u)\mathbf{S}^s\mathbf{P}_m^s(u'),\quad u,u'\in[-1,+1], \tag{10}$$

where

$$\mathbf{S}^s=\begin{bmatrix}a_1^s & b_1^s & 0 & 0\\ b_1^s & a_2^s & 0 & 0\\ 0 & 0 & a_3^s & b_2^s\\ 0 & 0 & -b_2^s & a_4^s\end{bmatrix}. \tag{11}$$

The elements of $\mathbf{S}^s$ are expansion coefficients since they follow from expansion of the elements of the scattering matrix

$$\mathbf{F}(\theta)=\begin{bmatrix}a_1(\theta) & b_1(\theta) & 0 & 0\\ b_1(\theta) & a_2(\theta) & 0 & 0\\ 0 & 0 & a_3(\theta) & b_2(\theta)\\ 0 & 0 & -b_2(\theta) & a_4(\theta)\end{bmatrix} \tag{12}$$

in terms of the generalized spherical functions $P_{mn}^s(\cos\theta)$; here,

$$a_1(\theta)=\sum_{s=0}^{\infty}a_1^sP_{00}^s(\cos\theta), \tag{13}$$

$$a_2(\theta)+a_3(\theta)=\sum_{s=2}^{\infty}(a_2^s+a_3^s)P_{22}^s(\cos\theta), \tag{14}$$

$$a_2(\theta)-a_3(\theta)=\sum_{s=2}^{\infty}(a_2^s-a_3^s)P_{2-2}^s(\cos\theta), \tag{15}$$

$$a_4(\theta)=\sum_{s=0}^{\infty}a_4^sP_{00}^s(\cos\theta), \tag{16}$$

$$b_1(\theta) = \sum_{s=2}^{\infty} b_1^s P_{02}^s(\cos\theta), \tag{17}$$

$$b_2(\theta) = \sum_{s=2}^{\infty} b_2^s P_{02}^s(\cos\theta), \tag{18}$$

θ is the scattering angle.

The matrices $\mathbf{P}_m^s$ occurring in Eq. (10) are defined as

$$\mathbf{P}_m^s(u) = \begin{bmatrix} P_{m0}^s(u) & 0 & 0 & 0 \\ 0 & P_{m+}^s(u) & P_{m-}^s(u) & 0 \\ 0 & P_{m-}^s(u) & P_{m+}^s(u) & 0 \\ 0 & 0 & 0 & P_{m0}^s(u) \end{bmatrix}, \tag{19}$$

where

$$P_{m\pm}^s(u) = \tfrac{1}{2}[P_{m-2}^s(u) \pm P_{m2}^s(u)]. \tag{20}$$

Convenient recurrence relations for computing generalized spherical functions $P_{mn}^s(u)$ are given in Refs. 2 and 4.

The matrices $\mathbf{Z}^m$ satisfy the symmetry relations[4]

$$\mathbf{Z}^m(u, u') = \mathbf{q}_4[\mathbf{Z}^m(u', u)]^{\mathrm{T}}\mathbf{q}_4, \tag{21}$$

$$\mathbf{Z}^m(-u, -u') = \mathbf{q}_3[\mathbf{Z}^m(u', u)]^{\mathrm{T}}\mathbf{q}_3, \tag{22}$$

where T denotes matrix transposition, and

$$\mathbf{q}_3 = \mathrm{diag}(1, 1, -1, 1), \tag{23}$$

$$\mathbf{q}_4 = \mathrm{diag}(1, 1, 1, -1). \tag{24}$$

In Sec. 3 and 4, we shall discuss the technique for calculating the matrices $\mathbf{R}^m$ by means of a numerical solution of Eq. (8). When the matrices $\mathbf{R}^m$ are computed, the intensity vector for the reflected light can be found through Eqs. (2)–(7).

3. NUMERICAL SOLUTION OF THE INVARIANT IMBEDDING EQUATION

Using a quadrature formula for numerical evaluation of the integrals in Eq. (8), we obtain the system of ordinary differential equations

$$\begin{aligned} \frac{\mathrm{d}\mathbf{R}^m(t;\mu_i,\mu_j)}{\mathrm{d}t} = & -\left(\frac{1}{\mu_i}+\frac{1}{\mu_j}\right)\mathbf{R}^m(t;\mu_i,\mu_j) + \frac{w}{4\mu_i\mu_j}\mathbf{Z}^m(-\mu_i,\mu_j) + \frac{w}{2\mu_j}\sum_{k=1}^{n_*}\mathbf{R}^m(t;\mu_i,\mu_k)\mathbf{Z}^m(\mu_k,\mu_j)w_k \\ & + \frac{w}{2\mu_i}\sum_{k=1}^{n_*}\mathbf{Z}^m(-\mu_i,-\mu_k)\mathbf{R}^m(t;\mu_k,\mu_j)w_k + w\sum_{k=1}^{n_*}\sum_{k'=1}^{n_*}\mathbf{R}^m(t;\mu_i,\mu_k)\mathbf{Z}^m(\mu_k,-\mu_{k'}) \\ & \times \mathbf{R}^m(t;\mu_{k'},\mu_j)w_k w_{k'}, \end{aligned} \tag{25}$$

where μ_k and w_k ($k = 1, \ldots, n_*$) are the division points and weights of the quadrature formula in the interval (0, 1), respectively. The initial condition is

$$\mathbf{R}^m(0;\mu_i,\mu_j) = \mathbf{R}^m(\mu_i,\mu_j). \tag{26}$$

Following Sato et al,[1] we rewrite Eq. (25) in the compact form

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{R}(t) = -C\mathbf{R}(t) + \mathbf{F}(t), \tag{27}$$

where

$$C = 1/\mu_i + 1/\mu_j, \tag{28}$$

$$\mathbf{R}(t) = \mathbf{R}^m(t;\mu_i,\mu_j), \tag{29}$$

$$\mathbf{F}(t) = w\mathbf{Z}^m(-\mu_i, \mu_j)/(4\mu_i\mu_j) + \frac{w}{2\mu_j}\sum_{k=1}^{n_*} \mathbf{R}^m(t; \mu_i, \mu_k)\mathbf{Z}^m(\mu_k, \mu_j)w_k$$

$$+ \frac{w}{2\mu_i}\sum_{k=1}^{n_*} \mathbf{Z}^m(-\mu_i, -\mu_k)\mathbf{R}^m(t; \mu_k, \mu_j)w_k$$

$$+ w\sum_{k=1}^{n_*}\sum_{k'=1}^{n_*} \mathbf{R}^m(t; \mu_i, \mu_k)\mathbf{Z}^m(\mu_k, -\mu_{k'})\mathbf{R}^m(t; \mu_{k'}, \mu_j)w_k w_{k'}. \quad (30)$$

Let the entire optical thickness of the atmosphere be t_*. Dividing the interval $[0, t_*]$ into subintervals $[0, t_1], \ldots, [t_{q-1}, t_*]$, setting $h_p = t_p - t_{p-1}$, $p = 1, \ldots, q$, and assuming $\mathbf{R}(t_{p-1})$ to be computed, we use the formal solution of Eq. (27) to compute[1]

$$\mathbf{R}(t_p) = \exp(-Ch_p)\mathbf{R}(t_{p-1}) + \int_{t_{p-1}}^{t_p} \exp[-C(t_p - t)]\mathbf{F}(t)\,\mathrm{d}t. \quad (31)$$

Then, approximating $\mathbf{F}(t)$ by a polynomial in t of degree S, viz.

$$\mathbf{F}(t) = \sum_{s=0}^{S} (t - t_{p-1})^s (s!h_p^s)^{-1}\mathbf{a}_s, \quad (32)$$

we may evaluate the integral in Eq. (31) analytically and obtain the correction formula

$$\mathbf{R}(t_p) = \exp(-Ch_p)\mathbf{R}(t_{p-1}) + \sum_{s=0}^{S} f_s\mathbf{a}_s, \quad (33)$$

where

$$f_0 = [1 - \exp(-Ch_p)]/C, \quad (34)$$

$$f_{s+1} = [1/(s+1)! - f_s/h_p]/C. \quad (35)$$

The matrices $\mathbf{a}_s$ are determined from the successive values $\mathbf{F}(t_{p-S}), \ldots, \mathbf{F}(t_p)$. We consider two special cases.

(i) $p = 1$. For this case, $S = 1$ and

$$\mathbf{F}(0) = \mathbf{a}_0, \quad \mathbf{F}(t_1) = \mathbf{a}_0 + \mathbf{a}_1; \quad (36)$$

from Eq. (33), we have

$$\mathbf{R}(t_1) = \exp(-Ch_1)\mathbf{R}(0) + (f_0 - f_1)\mathbf{F}(0) + f_1\mathbf{F}(t_1). \quad (37)$$

(ii) $p \geqslant 2$. For this case, $S = 2$. We determine the matrices $\mathbf{a}_0$, $\mathbf{a}_1$, and $\mathbf{a}_2$ from the system of equations

$$\mathbf{F}(t_{p-2}) = \mathbf{a}_0 - \mathbf{a}_1/d_p + \mathbf{a}_2/(2d_p^2),$$

$$\mathbf{F}(t_{p-1}) = \mathbf{a}_0, \quad \mathbf{F}(t_p) = \mathbf{a}_0 + \mathbf{a}_1 + \mathbf{a}_2/2, \quad (38)$$

where $d_p = h_p/h_{p-1}$. Finally, we have from Eq. (33)

$$\mathbf{R}(t_p) = \exp(-Ch_p)\mathbf{R}(t_{p-1}) + d_p^2(-f_1 + 2f_2)(1 + d_p)^{-1}\mathbf{F}(t_{p-2})$$

$$+ [f_0 + (d_p - 1)f_1 - 2d_pf_2]\mathbf{F}(t_{p-1}) + (f_1 + 2d_pf_2)(1 + d_p)^{-1}\mathbf{F}(t_p). \quad (39)$$

Equations (37) and (39) are systems of nonlinear equations and are solved by simple iterations. As an initial estimate for $p = 1$, we take

$$\mathbf{R}_{\mathrm{in}}(t_1) = \exp(-Ch_1)\mathbf{R}(0) + f_0\mathbf{F}(0). \quad (40)$$

For $p = 2$, we use the linear extrapolation

$$\mathbf{R}_{\mathrm{in}}(t_2) = \mathbf{R}(t_1) + [\mathbf{R}(t_1) - \mathbf{R}(0)]d_2. \quad (41)$$

For $p \geqslant 3$, we use the quadratic extrapolation

$$\begin{aligned}\mathbf{R}_{\text{in}}(t_p) = {} & \mathbf{R}(t_{p-3})(t_p - t_{p-2})(t_p - t_{p-1})/[(t_{p-3} - t_{p-2})(t_{p-3} - t_{p-1})] \\ & + \mathbf{R}(t_{p-2})(t_p - t_{p-3})(t_p - t_{p-1})/[(t_{p-2} - t_{p-3})(t_{p-2} - t_{p-1})] \\ & + \mathbf{R}(t_{p-1})(t_p - t_{p-3})(t_p - t_{p-2})/[t_{p-1} - t_{p-3})(t_{p-1} - t_{p-2})].\end{aligned} \tag{42}$$

The convergence criterion is

$$\max|[R^m_{nn'}(t_p; \mu_i, \mu_j)]_r - [R^m_{nn'}(t_p; \mu_i, \mu_j)]_{r-1}| < \Delta, \quad i, j = 1, \ldots, n_*; \ n, n' = 1, \ldots, 4 \tag{43}$$

where r is the iteration number for the pth integration step, and Δ is the required accuracy of the computations.

4. SOME COMPUTATIONAL ASPECTS

4.1. The azimuth-independent term

It follows from Eqs. (10), (11), (19), and (20) that the matrix $\mathbf{Z}^0$ is diagonal,[6] i.e.

$$\mathbf{Z}^0 = \begin{bmatrix} \mathbf{Z}_{IQ} & \mathbf{0} \\ \mathbf{0} & \mathbf{Z}_{UV} \end{bmatrix}. \tag{44}$$

Here, $\mathbf{0}$ is the (2×2) zero matrix and $\mathbf{Z}_{IQ}$ and $\mathbf{Z}_{UV}$ are (2×2) matrices given, respectively, by

$$\mathbf{Z}_{IQ}(u, u') = \sum_{s=0}^{\infty} \mathbf{P}^s_{01}(u)\mathbf{S}^s_1\mathbf{P}^s_{01}(u'), \tag{45}$$

$$\mathbf{Z}_{UV}(u, u') = \sum_{s=0}^{\infty} \mathbf{P}^s_{02}(u)\mathbf{S}^s_2\mathbf{P}^s_{02}(u'), \tag{46}$$

with

$$\mathbf{S}^s_1 = \begin{bmatrix} a^s_1 & b^s_1 \\ b^s_1 & a^s_2 \end{bmatrix}, \quad \mathbf{S}^s_2 = \begin{bmatrix} a^s_3 & b^s_2 \\ -b^s_2 & a^s_4 \end{bmatrix}, \tag{47}$$

$$\mathbf{P}^s_{01}(u) = \text{diag}[P^s_{00}(u), \ P^s_{02}(u)], \tag{48}$$

$$\mathbf{P}^s_{02}(u) = \text{diag}[P^s_{02}(u), \ P^s_{00}(u)]. \tag{49}$$

Assuming the matrix $\mathbf{R}^0(\mu, \mu_0)$ to be diagonal,

$$\mathbf{R}^0(\mu, \mu_0) = \begin{bmatrix} \mathbf{R}_{IQ}(\mu, \mu_0) & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{UV}(\mu, \mu_0) \end{bmatrix}, \tag{50}$$

we find from Eqs. (8), (9), and (44) that the matrix $\mathbf{R}^0(t; \mu, \mu_0)$ is also diagonal,

$$\mathbf{R}^0(t; \mu, \mu_0) = \begin{bmatrix} \mathbf{R}_{IQ}(t; \mu, \mu_0) & \mathbf{0} \\ \mathbf{0} & \mathbf{R}_{UV}(t; \mu, \mu_0) \end{bmatrix}. \tag{51}$$

Thus, instead of solving Eq. (8) for the (4×4) matrix $\mathbf{R}^0(t; \mu, \mu_0)$, we may solve two independent equations for the (2×2) matrices $\mathbf{R}_{IQ}(t; \mu, \mu_0)$ and $\mathbf{R}_{UV}(t; \mu, \mu_0)$. These equations are obtained from Eq. (8) by the substitutions

$$\mathbf{Z}^0 \to \mathbf{Z}_{IQ}, \quad \mathbf{R}^0 \to \mathbf{R}_{IQ}$$

and

$$\mathbf{Z}^0 \to \mathbf{Z}_{UV}, \quad \mathbf{R}^0 \to \mathbf{R}_{UV}.$$

Moreover, if the incident radiation is unpolarized or linearly polarized [i.e., if $\mathbf{F} = (F_I, 0, 0, 0)^{\mathrm{T}}$ or $\mathbf{F} = (F_I, F_Q, 0, 0)^{\mathrm{T}}$, respectively], we may solve only the equation for the matrix $\mathbf{R}_{IQ}$. As a result, the computational time and storage requirements are greatly reduced.

4.2. Symmetry relations

Assuming the matrix $\mathbf{R}^m(\mu, \mu_0)$ to satisfy the symmetry relation

$$\mathbf{R}^m(\mu, \mu_0) = \mathbf{q}_3[\mathbf{R}^m(\mu_0, \mu)]^{\mathrm{T}}\mathbf{q}_3 \tag{52}$$

and using Eqs. (8) and (22), we find that the matrix

$$\mathbf{R}_1^m(t; \mu, \mu_0) = \mathbf{q}_3[\mathbf{R}^m(t; \mu_0, \mu)]^{\mathrm{T}}\mathbf{q}_3$$

is also a solution of Eq. (8) subject to the initial condition

$$\mathbf{R}_1^m(0; \mu, \mu_0) = \mathbf{R}^m(\mu, \mu_0).$$

Therefore, assuming uniqueness of the solution of Eqs. (8), (9), we obtain the symmetry relation

$$\mathbf{R}^m(t; \mu, \mu_0) = \mathbf{q}_3[\mathbf{R}^m(t; \mu_0, \mu)]^{\mathrm{T}}\mathbf{q}_3. \tag{53}$$

Using this symmetry relation, we can reduce the number of equations in Eqs. (25) by the factor $2n_*/(n_* + 1)$.

For the special case $m = 0$, we have

$$\begin{aligned} \mathbf{R}_{IQ}(t; \mu, \mu_0) &= [\mathbf{R}_{IQ}(t; \mu_0, \mu)]^{\mathrm{T}}, \\ \mathbf{R}_{UV}(t; \mu, \mu_0) &= \mathbf{q}_3'[\mathbf{R}_{UV}(t; \mu_0, \mu)]^{\mathrm{T}}\mathbf{q}_3' \end{aligned} \tag{54}$$

where $\mathbf{q}_3' = \mathrm{diag}(-1, 1)$.

4.3. Diagonalization of the matrices $\mathbf{P}_m^s(u)$

In actual computations, diagonalization of the matrices $\mathbf{P}_m^s(u)$ for $m > 0$ is useful.[4,5] We write

$$\mathbf{P}_m^s(u) = \mathbf{S}\mathbf{R}_m^s(u)\mathbf{S}, \tag{55}$$

where

$$\mathbf{S} = \mathbf{S}^{\mathrm{T}} = \mathbf{S}^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{56}$$

$$\mathbf{R}_m^s(u) = \mathrm{diag}[P_{m0}^s(u), P_{m-2}^s(u), P_{m2}^s(u), P_{m0}^s(u)]. \tag{57}$$

Then

$$\mathbf{Z}^m(u, u') = (-1)^m\mathbf{S}\left\{\sum_{s=m}^{\infty} \mathbf{R}_m^s(u)[\mathbf{S}\mathbf{S}^s\mathbf{S}]\mathbf{R}_m^s(u')\right\}\mathbf{S}. \tag{58}$$

4.4. Supermatrices

Following Refs. 2 and 7, we define

$$[\mathbf{Z}_{\pm\pm}^m]_{N(i-1)+p,N(j-1)+q} = \sqrt{w_i w_j}\, Z_{pq}^m(\pm\mu_i, \pm\mu_j), \tag{59}$$

$$[\mathbf{R}^m(t)]_{N(i-1)+p,N(j-1)+q} = \sqrt{w_i w_j}\, R_{pq}^m(t; \mu_i, \mu_j), \tag{60}$$

$$[\mathbf{C}]_{N(i-1)+p,N(j-1)+q} = \frac{1}{\mu_i}\delta_{ij}\delta_{pq}, \tag{61}$$

$$[\mathbf{Q}_3]_{N(i-1)+p,N(j-1)+q} = (1 - 2\delta_{p3})\delta_{ij}\delta_{pq}, \tag{62}$$

$$[\mathbf{Q}_4]_{N(i-1)+p,N(j-1)+q} = (1 - 2\delta_{p4})\delta_{ij}\delta_{pq}, \tag{63}$$

where $i, j = 1, \ldots, n_*$, $p, q = 1, \ldots, N$, and N is in general equal to 4. The matrices $\mathbf{Z}_{\pm\pm}^m$ and $\mathbf{R}^m(t)$ are called supermatrices and are composed of n_*^2 matrices of dimension $(N \times N)$. From Eqs. (21), (22), and (53), we obtain the symmetry relations

$$\mathbf{Z}_{\pm\pm}^m = \mathbf{Q}_4[\mathbf{Z}_{\pm\pm}^m]^{\mathrm{T}}\mathbf{Q}_4, \tag{64}$$

Table 1. The expansion coefficients for the Rayleigh scattering matrix.

s	a_1^s	a_2^s	a_3^s	a_4^s	b_1^s	b_2^s
0	1	0	0	0	0	0
1	0	0	0	3/2	0	0
2	1/2	3	0	0	$\sqrt{3/2}$	0

Table 2. Computational parameters.

m	N	h_1	d
0	2	0.03	1.03
1	3	0.04	1.04
2	3	0.05	1.05

$$\mathbf{Z}^m_{\pm\pm} = \mathbf{Q}_3[\mathbf{Z}^m_{\mp\mp}]^{\mathrm{T}}\mathbf{Q}_3, \tag{65}$$

$$\mathbf{R}^m(t) = \mathbf{Q}_3[\mathbf{R}^m(t)]^{\mathrm{T}}\mathbf{Q}_3. \tag{66}$$

Using the definitions of Eqs. (59)–(63), we rewrite the invariant imbedding equation in the form

$$\frac{\mathrm{d}\mathbf{R}^m(t)}{\mathrm{d}t} = -\mathbf{C}\mathbf{R}^m(t) - \mathbf{R}^m(t)\mathbf{C} + \frac{w}{4}\mathbf{C}\mathbf{Z}^m_{-+}\mathbf{C} + \frac{w}{2}\mathbf{R}^m(t)\mathbf{Z}^m_{++}\mathbf{C} + \frac{w}{2}\mathbf{C}\mathbf{Z}^m_{--}\mathbf{R}^m(t) + w\mathbf{R}^m(t)\mathbf{Z}^m_{+-}\mathbf{R}^m(t). \tag{67}$$

Thus, the angle integration and the (4×4) matrix multiplication in Eq. (8) are replaced by the single multiplication of supermatrices in Eq. (67), which is advantageous for computational purposes.[2,7]

By changing the value of N, several important particular cases can be considered. First, setting $N = 1$, we calculate the scalar reflection function.[1] Then, using the value $N = 2$ for $m = 0$, we calculate the matrix $\mathbf{R}_{IQ}$. Finally, setting $N = 3$ for $m \geqslant 1$, we calculate the matrices $\mathbf{R}^m$ in the 3×3 approximation.[8]

4.5. *Varying the size of integration steps*

Sato et al[1] have noted that an important feature of the fast invariant imbedding method is the possibility of varying the size of successive integration steps $h_p = t_p - t_{p-1}$. The simplest way for choosing the value of h_p is to set $h_p = dh_{p-1}$ for $t_{p-1} < t_*/2$ with $d > 1$, and to set $h_p = h_{p-1}/d$ for $t_{p-1} > t_*/2$. Thus, approaching the upper boundary of the atmosphere, we decrease the size of the integration steps and, therefore, increase the accuracy of the computations for the upper atmospheric layers that most significantly affect the Stokes parameters of the reflected light.

Table 3. Stokes parameters of the reflected light for $\mu_0 = 0.9$, $\varphi_0 = 0°$, and $g = 0$.

μ	I			Q			U
	φ=0°	φ=90°	φ=180°	φ=0°	φ=90°	φ=180°	φ=90°
0.05	0.3946	0.3591	0.4153	-0.1993	-0.1428	-0.1786	-0.2063
0.1	0.3889	0.3647	0.4295	-0.2022	-0.1364	-0.1616	-0.2030
0.2	0.3671	0.3645	0.4434	-0.2035	-0.1213	-0.1272	-0.1906
0.3	0.3390	0.3551	0.4430	-0.1987	-0.1037	-0.0946	-0.1734
0.4	0.3113	0.3424	0.4346	-0.1887	-0.0849	-0.0655	-0.1541
0.5	0.2881	0.3302	0.4224	-0.1750	-0.0659	-0.0406	-0.1343
0.6	0.2708	0.3198	0.4084	-0.1580	-0.0472	-0.0205	-0.1146
0.7	0.2602	0.3119	0.3929	-0.1379	-0.0289	-0.0052	-0.0948
0.8	0.2567	0.3064	0.3752	-0.1139	-0.0111	0.0045	-0.0740
0.9	0.2625	0.3029	0.3528	-0.0838	0.0062	0.0066	-0.0502
1.0	0.3014	0.3014	0.3014	-0.0232	0.0232	-0.0232	-0.0000

Table 4. As in Table 3, for $g = 0.001$.

μ	I			Q			U
	$\varphi=0°$	$\varphi=90°$	$\varphi=180°$	$\varphi=0°$	$\varphi=90°$	$\varphi=180°$	$\varphi=90°$
0.05	0.3945	0.3589	0.4151	-0.1992	-0.1428	-0.1786	-0.2063
0.1	0.3887	0.3645	0.4293	-0.2021	-0.1364	-0.1615	-0.2029
0.2	0.3668	0.3643	0.4430	-0.2034	-0.1213	-0.1272	-0.1905
0.3	0.3387	0.3548	0.4427	-0.1986	-0.1037	-0.0946	-0.1733
0.4	0.3110	0.3421	0.4343	-0.1887	-0.0849	-0.0654	-0.1540
0.5	0.2878	0.3298	0.4221	-0.1749	-0.0659	-0.0406	-0.1343
0.6	0.2706	0.3195	0.4080	-0.1579	-0.0472	-0.0205	-0.1146
0.7	0.2599	0.3116	0.3925	-0.1378	-0.0289	-0.0052	-0.0947
0.8	0.2564	0.3061	0.3748	-0.1139	-0.0111	0.0045	-0.0740
0.9	0.2622	0.3027	0.3525	-0.0837	0.0062	0.0065	-0.0502
1.0	0.3011	0.3011	0.3011	-0.0232	0.0232	-0.0232	-0.0000

Table 5. As in Table 3, for $g = 0.01$.

μ	I			Q			U
	$\varphi=0°$	$\varphi=90°$	$\varphi=180°$	$\varphi=0°$	$\varphi=90°$	$\varphi=180°$	$\varphi=90°$
0.05	0.3928	0.3573	0.4134	-0.1990	-0.1427	-0.1784	-0.2059
0.1	0.3867	0.3625	0.4272	-0.2018	-0.1363	-0.1614	-0.2024
0.2	0.3644	0.3618	0.4403	-0.2030	-0.1211	-0.1270	-0.1898
0.3	0.3361	0.3521	0.4396	-0.1980	-0.1035	-0.0945	-0.1726
0.4	0.3084	0.3393	0.4310	-0.1880	-0.0847	-0.0654	-0.1533
0.5	0.2853	0.3271	0.4188	-0.1742	-0.0658	-0.0407	-0.1336
0.6	0.2681	0.3168	0.4048	-0.1573	-0.0471	-0.0206	-0.1139
0.7	0.2575	0.3090	0.3894	-0.1372	-0.0289	-0.0053	-0.0942
0.8	0.2542	0.3035	0.3718	-0.1133	-0.0111	0.0044	-0.0735
0.9	0.2600	0.3002	0.3497	-0.0833	0.0062	0.0064	-0.0498
1.0	0.2987	0.2987	0.2987	-0.0231	0.0231	-0.0231	-0.0000

Table 6. As in Table 3, for $g = 0.1$.

μ	I			Q			U
	$\varphi=0°$	$\varphi=90°$	$\varphi=180°$	$\varphi=0°$	$\varphi=90°$	$\varphi=180°$	$\varphi=90°$
0.05	0.3777	0.3427	0.3980	-0.1970	-0.1416	-0.1768	-0.2022
0.1	0.3686	0.3449	0.4081	-0.1989	-0.1348	-0.1594	-0.1976
0.2	0.3422	0.3395	0.4155	-0.1984	-0.1191	-0.1251	-0.1833
0.3	0.3123	0.3275	0.4115	-0.1923	-0.1014	-0.0930	-0.1654
0.4	0.2847	0.3140	0.4016	-0.1816	-0.0829	-0.0647	-0.1462
0.5	0.2623	0.3019	0.3892	-0.1675	-0.0643	-0.0406	-0.1269
0.6	0.2461	0.2921	0.3757	-0.1507	-0.0461	-0.0211	-0.1080
0.7	0.2364	0.2849	0.3611	-0.1310	-0.0283	-0.0063	-0.0891
0.8	0.2336	0.2801	0.3447	-0.1079	-0.0111	0.0032	-0.0695
0.9	0.2395	0.2773	0.3241	-0.0791	0.0056	0.0055	-0.0470
1.0	0.2764	0.2764	0.2764	-0.0219	0.0219	-0.0219	-0.0000

Table 7. As in Table 3, for $g = 1.0$.

μ	I			Q			U
	φ=0°	φ=90°	φ=180°	φ=0°	φ=90°	φ=180°	φ=90°
0.05	0.2986	0.2673	0.3163	-0.1788	-0.1296	-0.1611	-0.1770
0.1	0.2733	0.2528	0.3061	-0.1728	-0.1187	-0.1399	-0.1643
0.2	0.2288	0.2259	0.2850	-0.1600	-0.0984	-0.1039	-0.1404
0.3	0.1947	0.2049	0.2665	-0.1468	-0.0801	-0.0749	-0.1197
0.4	0.1695	0.1893	0.2510	-0.1332	-0.0635	-0.0517	-0.1018
0.5	0.1518	0.1780	0.2378	-0.1192	-0.0483	-0.0332	-0.0860
0.6	0.1402	0.1703	0.2263	-0.1047	-0.0342	-0.0187	-0.0717
0.7	0.1338	0.1652	0.2154	-0.0893	-0.0211	-0.0077	-0.0583
0.8	0.1324	0.1623	0.2043	-0.0723	-0.0087	-0.0004	-0.0449
0.9	0.1369	0.1610	0.1911	-0.0522	0.0031	0.0020	-0.0301
1.0	0.1611	0.1611	0.1611	-0.0144	0.0144	-0.0144	-0.0000

5. NUMERICAL RESULTS

In this section, we present some numerical results for the classical problem of Rayleigh scattering. For this particular case, the scattering matrix is

$$\mathbf{F}_{\mathrm{R}}(\theta) = \frac{3}{4}\begin{bmatrix} 1+\cos^2\theta & -\sin^2\theta & 0 & 0 \\ -\sin^2\theta & 1+\cos^2\theta & 0 & 0 \\ 0 & 0 & 2\cos\theta & 0 \\ 0 & 0 & 0 & 2\cos\theta \end{bmatrix}. \tag{68}$$

The values of the expansion coefficients are listed in Table 1.

As an example, we consider a slab with optical thickness $t_* = 1$ at the top of a perfectly absorbing ground. In Tables 3–7, we give numerical results for unpolarized incident light $\mathbf{F} = (1, 0, 0, 0)^{\mathrm{T}}$, and for the single scattering albedo of the form

$$w = \exp(-g\tau), \tag{69}$$

where the optical depth τ is measured from the upper boundary of the slab. We have used a Gaussian quadrature with $n_* = 20$ division points. Computational parameters N (see Sec. 4.4), h_1 and d (see Sec. 4.5) are listed in Table 2.

Our program was tested by comparing our results with those of Garcia and Siewert,[9] Viik,[10] and Maiorino and Siewert.[11] In Ref. 9, numerical results are given for inhomogeneous, isotropically-scattering atmospheres (scalar case) with an exponentially-varying single scattering albedo [cf. Eq. (69)]. In Refs. 10 and 11, results are given for homogeneous, Rayleigh-scattering atmospheres (the vector case). For all of these cases, we have found excellent agreement.

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